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INTERACTION: PART I
THEORETICAL PREDICTION OF MOMENTUM
AND ENERGY ACCOMMODATION FOR
HYPERVELOCITY GAS PARTICLES ON AN
IDEAL CRYSTAL SURFACE

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RESEARCH ON MOLECULE-SURFACE INTERACTION

PART I

THEORETICAL PREDICTION OF MOMENTUM AND
ENERGY ACCOMMODATION FOR HYPERVELOCITY
GAS PARTICLES ON AN IDEAL CRYSTAL SURFACE

by

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September 1964

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Director of Research

FOREWORD

This document is the first part of a three part final report on NASA contract number NASw-709. This part was originally presented at the Fourth International Symposium on Rarefied Gas Dynamics, Toronto, July 1964. It describes theoretical work under the above contract, which is a successor to NASr-104 on the same subject, namely, the interaction of high energy gas particles with solid surfaces.

This research was performed under the technical supervision of the NASA Physics of Fluids Office, Mr. Alfred P. Gessow, Chief. It covers the period from July 1, 1963 to August 9, 1964.

ABSTRACT

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Results from a system of calculations of the three dimensional interactions of gas molecules with ideal FCC surfaces are presented for a wide range of input conditions. One group of these calculations is set up according to a balanced statistical design, another deals with noble gases on a nickel surface. The model used is one previously described by Oman, Bogan, Weiser, and Li (1963). A Lennard-Jones 6-12 potential is assumed between the lattice atoms and the gas particles. The model is applicable only when the gas particle energy is very much greater than that corresponding to the lattice temperatures. Classical mechanics is used in the calculations; the gas particles are approximated by point masses; and both independent and coupled oscillators are evaluated for use in the lattice dynamics. The computations are carried out using an IBM 7094 computer. Interpretations of the results employ both statistical techniques and analysis of interactions between specific gas and solid species.

In this paper particular attention is devoted to the validity of approximating the lattice by a system of independent forced harmonic oscillators (i.e., an Einstein lattice). Comparison with a lattice model which includes coupling between atoms has shown that the independent oscillator model predicts the gas particle final state with sufficient accuracy for most purposes, especially

when the number of lattice vibrations during a collision is either large or small compared to unity.

Calculations of interactions of A, Ne, and He on a (100) Ni surface are presented for two incident angles and four incident energies from 0.125 to 8 ev. Statistical correlations are also presented for 12 different properties of the exit distributions in terms of the 6 independent nondimensional parameters which describe the incident state. Special behavior of certain molecular trajectories showing characteristics of adsorbed final states is also discussed.

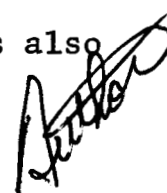


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I. INTRODUCTION

In a previous paper [Oman, Bogan, Weiser, and Li (1963)] a theoretical model and some sample results for a calculation of gas molecule interactions with crystal surfaces was presented. We have since investigated the effects of one of the most important assumptions in that model, namely independent lattice atoms, and used the model to make a comprehensive study by calculating a very large number of molecular trajectories covering a wide range of incident conditions. This paper discusses these recent investigations and presents the results in terms of mean interaction parameters and other statistical properties of the molecular distribution. Results are also given for several rare gases on Ni surfaces to show energy and geometry dependence for specific species.

Our theoretical model is set up with the specific application of hypervelocity flight in mind. We have sacrificed a detailed knowledge of the lattice processes after the interval during which they can affect the gas particle and have ignored the initial thermal motions in the lattice. These simplifications have made possible a more general and complete three dimensional description of the histories of the gas particles, including collisions which are arbitrarily oriented relative to the surface atoms.

There are several recent examples of theoretical methods which attack these problems from different viewpoints. Cabrera (1959), Zwanzig (1960), and McCarroll and Ehrlich (1963) employ lattice models consisting of one dimensional chains of atoms with linear restoring forces. They use different intermolecular force laws to show the effects of dispersion forces and lattice dynamics in transmitting energy to the lattice and in trapping the incident gas particles. Goodman (1962, 1963) has worked with one, two, and three dimensional lattice models and has concluded that the three dimensional case is qualitatively very different from the others. He considers a Morse potential between the gas particle and a single surface atom. Only head-on collisions at normal incidence are accounted for. Using a perturbation method, he has been able to solve the lattice dynamics for the realistic case of coupled oscillators.

All of the above authors ignore thermal motions in the lattice before impact. They also limit their consideration to the energy accommodation coefficient, making no attempt to predict momentum accommodation. These theories all use classical mechanics, an assumption which seems reasonable for incident energies above 0.1 ev with most gases (we discussed this point in our first paper) and enables one to employ a much more detailed physical model. Earlier quantum-mechanical treatments [cf. Devonshire (1937)] were forced by difficult mathematics to simplify the problem more drastically.

A recent work which takes a different approach is that of Marsh (1963). He treats the case in which thermal motions of the lattice dominate the interaction and relates the energy exchange to the time spent in residence on the surface. In his treatment the incident energy is not large compared to either the adsorption or lattice thermal energies (i.e., a colder gas on a hotter surface). He also presents a model for the treatment of accommodation of the internal degrees of freedom of the gas molecule which may prove to be adaptable to other cases as well.

Several points of agreement among these papers and our own work can be seen in the qualitative descriptions of the interaction processes. We will state the more important of these and indicate those authors that have in one way or another advanced similar arguments or results. These points were mentioned in our first paper and are reinforced by the present results.

1. Three dimensional lattices are fundamentally different from one or two dimensional ones.
For example, $\alpha_{1D} \rightarrow 1$ while $\alpha_{3D} \rightarrow 0$ as $\omega_n \tau_c \rightarrow \infty$. (Goodman; McCarroll and Ehrlich to some extent.)
2. The repulsive portion of the interaction potential is usually much more important to the energy exchange than the attractive portion. The attractive portion plays an important role in trapping

(which can itself produce high energy exchange) and in "guiding" the gas particle to a preferential site on the surface, but in most cases it is the maximum value of the interaction force that determines the energy exchange. (Goodman; McCarroll and Ehrlich.)

3. One or two surface atoms play a predominant role in the energy exchange process. This can also be seen from the steepness of the repulsive potential and from item 2 above. (Goodman.)
4. Head-on impacts with a surface atom will be relatively infrequent and often quite different from the more common glancing collisions, but analysis of the former can be helpful in characterizing the types of behavior to expect. (Goodman; McCarroll and Ehrlich.)

Many of the foregoing conclusions support the idealizations which were employed in our first paper for the formulation of similarity variables to be used in the correlation of energy accommodation coefficients. Although we do not discuss that approach in the present paper, we have continued along those lines as well. We feel that further work is required before the scatter in these correlations can be reduced to a level which justifies the labor involved in their use.

In dealing with gas-surface interactions on a molecular scale the formulation of a theoretical model and the carrying out of calculations for a small number of typical cases is only the beginning. There are a formidable number of possibilities represented in any model which attempts to present a moderately realistic picture of a three dimensional interaction. Even making use of nondimensional groups to reduce the number of variables, our model requires six independent variables in addition to the specification of the lattice type and surface plane [e.g., (100) face of a FCC lattice]. Most of these parameters can vary continuously over wide ranges within the regions of interest, and each of them can have a strong effect on the results. Furthermore, we have made no attempts to include surface roughness, adsorbed gases or other impurities, effects of internal degrees of freedom, electronic interactions, sputtering, or chemical effects. Numerical calculations of the type we are dealing with here usually cannot be performed each time information about specific situations is required. It is therefore very important to devote a corresponding effort to the systematic correlation and interpretation of the results. Two different approaches to the over-all problem will be shown; these are statistical design and data analysis, and the treatment

of specific gas and solid species. First, however, we shall review the calculation method and show the results of an investigation of the effects of energy propagation within the lattice during the interaction.

II. THEORETICAL MODEL

We have chosen a classical model employing the Lennard-Jones 6-12 potential (see Fig. 1) to represent the molecule-surface interaction. We approximate the solid by a lattice of potential sources, each bound to its original position by a linear restoring force, and each interacting only with the gas particle. The collision of an incident gas particle with a solid surface is then formulated in a manner such that its solution is amenable to high speed computer techniques.

The form of model for the interaction forces between the gas particle and the solid depends upon the distance between the particle and the solid surface. When the gas particle is a large distance from the lattice, greater than 5 lattice spacings, we use a closed form expression for the effect of the L-J potential from a semi-infinite continuum solid on a gas particle trajectory originating at infinity to account for the van der Waals (r^{-3}) attraction of the gas particle to the surface. For intermediate distances from the surface, 2.5 to 5 lattice spacings, we calculate the force on gas particle by a composite potential and assume that the lattice atoms do not move. The composite potential is the sum of a continuum potential (essentially van der Waals) and the L-J 6-12 potential from all the atoms in the lattice block minus a "pseudo-continuum" potential from the lattice block. The "pseudo-continuum" poten-

tial is the contribution of the solid in the lattice block to the van der Waals potential. Thus, the composite potential represents the potential from a semi-infinite continuum from which a block has been removed and filled with a discrete lattice of atoms (see Fig. 2). When the gas particle is very near the surface, closer than 2.5 lattice spacings, we consider the gas particle to interact only with each of the nearby atoms in the lattice via the L-J potential.

In the last two regimes we integrate the classical equations of motion of the gas particle numerically using the Runge-Kutta procedure. In the closest region, at each time step of the particle trajectory integration we calculate a new location for each lattice atom assuming the atom is bound to a fixed site by a linear restoring force and also under the influence of the L-J potential. We approximate the time-dependent L-J force by the first two terms in a Taylor series in time and insert this force into a closed form solution for the motion of a three dimensional harmonic oscillator under the influence of a linear (in time) external force. Since the mass of the lattice atom is almost always larger than the mass of the gas particles under consideration, the acceleration of the lattice particles will be smaller than the acceleration of the gas particle. The control of the time increment in the Runge-Kutta integration procedure which assures uniform accuracy for the calculation of

position on the gas trajectory also assures us that the time increment is small enough for this approximation to be valid. It is, of course, the motion of the lattice atoms which makes the potential field experienced by the gas particle nonconservative and is in this model the only source of energy transfer to the lattice.

One of the parameters governing the interaction is the exact point on the crystal surface structure where the gas particle interacts most strongly. The effect of this point of impact on the gas trajectory is large, but no particular point of impact corresponds to a definite physical condition in an actual molecular stream. Therefore, we have chosen to calculate average interaction parameters which represent the results of many trajectories for the same physical conditions (e.g., species of atom, angle of incidence, and energy). We choose our points of impact by distributing the aiming point uniformly over a repetitive area on the crystal surface and averaging the results for each physical state.

Our calculations are performed on an IBM 7094 computer. A schematic diagram of the computer logic is shown in Fig. 3. A typical single molecular trajectory requires about 1 minute of calculation time. We have chosen our lattice to be originally at rest. Hence, each calculation is completely deterministic

and the ratio E_ℓ/E_i , where E_ℓ is the energy of the lattice at the end of the calculation and E_i is the initial energy of the gas particle, corresponds to the thermal accommodation coefficient. A check on the accuracy is always available in the conservation of energy and we find that most runs have discrepancies of less than 2 per cent.

III. COMPARISON OF TWO LATTICE MODELS

One of the most questionable of our assumptions is the model for the lattice dynamics. Since each lattice atom is assumed to be bound to a fixed site, the propagation of energy by lattice waves is precluded. The assessment of the limits of validity of this model, which we call the independent oscillator lattice (IOL), is one of the major goals of this paper.

In order to evaluate the IOL approximation we have set up a second lattice model which we call the coupled oscillator lattice (COL). In the COL, each lattice atom is bound by a linear restoring force to the center of gravity of the location of its nearest neighbors at the end of the previous time interval. This method allows for the propagation of lattice waves but, unfortunately, requires about 10 times as much computer time as the IOL to get acceptably accurate solutions.

We have calculated individual trajectories in pairs that have corresponding initial conditions for comparison of the IOL and the COL. The values of the independent variables for these

comparisons were chosen from a balanced fractional design, the purpose of which is to cover all parts of the independent variable space uniformly and efficiently with a small number of tests. A few additional runs were added to these cases to display the effects of extreme values of certain independent variables. In Fig. 4 (a-d) we have shown the results of these comparisons in the form of differences between the various interaction parameters for corresponding cases. There is no correlation to these points, nor should one be expected, as they represent varying values of six different independent variables. The abscissa of the plot is $\omega_n \tau_c$, the product of the natural frequency of the lattice and an estimated collision duration which is calculated from the independent variables. This timing parameter is the most important factor in controlling the validity of the IOL approximation. A formula for approximating $\omega_n \tau_c$ is derived in our first paper by considering an equivalent frequency ω_c for the interaction force. This expression becomes:

$$\frac{\omega_c}{\omega_n} = (\omega_n \tau_c)^{-1} = \frac{\pi}{2} \frac{\sin \theta_i}{\Omega(\sigma/d)} \left[2^{\frac{1}{3}} - \left(\frac{2}{1 + \sqrt{1 + \frac{\cos^2 \theta_i}{D_w}}} \right)^{\frac{1}{3}} \right]^{-\frac{1}{2}} \quad (1)$$

where

$$\Omega = \omega_n \frac{d}{v_i}$$

One might expect that the IOL approximation would break down as $\omega_n \tau_c$ became large. In one sense this does occur, because the energy transmitted to the COL can amount to two or three times E_ℓ for the IOL. However, it is also true that E_ℓ/E_i approaches zero quite rapidly as $\omega_n \tau_c$ gets large, and the difference in E_ℓ between models also vanishes when compared to the total energy of the system (E_i). The largest differences in final gas-particle energy occur for $1 < \omega_n \tau_c < 10$, which is to be expected from the above discussion. A single pair of runs, having a value of nondimensional binding energy ($D_w = \epsilon/E_i$) larger than those employed in our other work, has a significantly larger difference in energy than the rest of the trials.

The comparisons of momentum accommodation (Fig. 4, b and c) show a moderate effect of the difference in lattice model, but practically all of this effect can be attributed to the change in exit velocity which is in turn related to the change in energy accommodation. Figure 4d shows this by a display of the changes in exit angles for corresponding cases. These are only a few degrees and can probably be ignored for most purposes.

This partial agreement between the two lattice models means that the IOL is a useful tool for many purposes, even for values of $\omega_n \tau_c$ much larger than unity. For calculations in which the effect of the surface interaction on the flow is the quantity of interest, the IOL model is adequate throughout the dynamic range. If the energy delivered to the surface per molecular impact is desired, the IOL will overestimate E_ℓ significantly if $\omega_n \tau_c > 5$. Since this corresponds to low E_ℓ/E_i , we have concluded that there is no advantage in employing the COL with our type of calculation. The numerical uncertainties will often represent 1 per cent of E_i , so we can never give very dependable numbers for E_ℓ/E_i when it is itself of that order. We have therefore employed the IOL for all of the calculations discussed in the remainder of this paper.

IV. STATISTICAL ANALYSIS

We have applied the methods of statistics to the design and analysis of our computer runs. Very briefly,^{*} the basic scheme of such methods is to distribute a relatively small number of trials over the very many possible combinations of independent (input) variables in a uniform, balanced fashion. In each computer run several input variables are simultaneously changed according to a prescribed plan; we deliberately avoid "varying one thing at a time." The results of the calculations are then

*

See, for example Fisher (1953) or Davies (1956) for more information on these techniques.

subjected to variance and regression analyses, from which a large number of statistical properties and coefficients can be extracted. Only the most important of these are given in this paper.

The design is balanced so that we can efficiently and accurately estimate the separate and combined effects of the six input variables for each dependent variable [cf. Davies (1956)]. We selected a pattern of 64 trials (out of a possible 512) designed to give equal weight to high, intermediate, and low values of each of the independent variables. Furthermore, this plan has the valuable feature that it is also balanced for the first 16 or 32 runs. This feature allowed a small-scale trial of the method with the option of either stopping or expanding. At each stopping point there is enough information to perform efficient statistical analyses.

We have chosen to distribute our trials over four levels of three input parameters Ω^2 , D_w , and θ_i . Two levels were used for each of the remaining parameters, σ/d , m_ℓ/m_g and φ_i . Table I gives these levels, which were chosen to represent the ranges of interest in hypervelocity flight. The center of the experimental region, the reference point for correlation coefficients, is also given in Table I. Logarithmic values are used in the correlations for m_ℓ/m_g , D_w , and Ω^2 .

The thermal accommodation coefficient is given by E_ℓ/E_i in our model and is calculated from the gas particle final energy by $E_\ell/E_i = 1 - E_f/E_i$. The standard deviations and means are taken over the 18 individual trajectories that represent a given incident state. The standard deviation is very closely related to the temperature of the exit distribution for the case of exit energy, and is a measure of the width of the exit distribution.

We have presented two of the many possible types of correlation from our statistical analyses. We selected these on the basis of their usefulness. The first type is a "best fitting" estimation equation for each of the dependent variables of interest. This equation consists of a superposition of least square linear trends for each of the independent variables, with quadratic correction terms added when a sufficient number of test levels was available to allow their calculation. This equation can be expressed in the following form:

$$\alpha_k = \bar{\alpha}_k + \sum_{j=1}^6 A_{kj}(x_j - \bar{x}_j) + \sum_{j=1}^3 B_{kj}(x_j - \bar{x}_j)^2 \quad k = 1, 10 \quad (2)$$

where α_k is a generalized property of the distribution of exit molecular states, $\bar{\alpha}_k$ its mean over all of the trials, A_{kj} the linear regression coefficient, B_{kj} the quadratic term coefficient. In Eq. (2) x_j denotes a particular input variable (or

its natural logarithm) and \bar{x}_j is the corresponding coordinate of the center of the experimental region. Values of coefficients [A] and [B] for the means and standard deviations of several interaction parameters are presented in Table II. Significance levels from the variance analysis are also indicated for each of the coefficients in Table II by a three-level code (blank, value, value and asterisk representing respectively < 90%, 90-99%, and 99.9% significance level). These significance levels measure how well the indicated correlations fit the data.

In addition to the formal calculation of statistical significance, there is available to us in this instance a simple over-all test of these correlations. We have compared the values for interaction parameters predicted by the correlation of Table II to the actual cases calculated in the computer (from which the fits were originally calculated). We feel the resulting discrepancies are the best simple measure of the "noise" in our statistical correlations. For E_ℓ/E_i this standard error of estimation (i.e., the standard deviation of the discrepancy over the computed results for 64 runs), was 0.109, compared to a mean E_ℓ/E_i of 0.4662. For σ_z the standard error was 0.187 on a mean of 1.7858, and for σ_T it was 0.188 on a mean of 0.6115. We also tested the same correlation with the 19 runs using specific species (in which many of the input ranges were extrapolated, particularly the mass ratio). These test cases are independent of those which generated

the correlation. The corresponding numbers for those cases were 0.082/0.5235, 0.254/1.5995, and 0.234/0.4639; for E_ℓ/E_i , σ_z , and σ_T , respectively. For these comparisons E_ℓ/E_i was set equal to zero or unity in the rare cases when these limits were exceeded. A comparison of predicted [i.e., from Table II and Eq. (2)] and calculated values of E_ℓ/E_i are shown in Fig. 5. The runs shown include the basic 64 in addition to the 19 runs described in the following discussion.

The second type of correlation is an expression of the mutual dependence of different properties of independent molecular trajectories within a given run. In particular, we are in this instance relating the amount of energy exchange to the direction of the exit ray. An examination of significance levels for many different types of these (i.e., output vs. output) correlations indicates that the most significant relationship is between E_f and the absolute magnitude of the polar angle measured from the specular ray, ψ . (This useful angle and its standard deviation have been calculated for each computer run, and their correlations are given in Table II.) As expected, and noted from preliminary indications in our first paper, there is a strong (but noisy) correlation, such that E_f decreases as the gas particle is scattered further from the specular direction. These 64 correlation coefficients naturally vary widely for different input states within our 64 runs, but the mean trend is -0.0030 E_i/degree .

V. DISCUSSION OF RESULTS

The general characteristics of typical molecular trajectories calculated for the IOL model were discussed in our first paper. In this paper we discuss a few situations which have special behavior, and indicate those trends which we have thus far detected in the data. There are two basic groups of runs: the statistically planned design described in Section IV, in which dynamic parameters are independently varied; and sets of specific-species interactions in which the relationships between some of the parameters are prescribed by the physical properties of the substances involved. In the latter case we have dealt with inert gases on a nickel surface. It is encouraging to note that the major trends indicated by the different approaches are in quite good agreement.

A. TRAPPING

There are several conditions for which our computer program is unable to provide a final exit velocity vector for the gas molecule. They usually arise from the demand for an excessive number of calculation intervals, resulting in a build-up of total error in the calculations to the point where we consider them

meaningless and/or excessively expensive, and the calculation is stopped. Other direct causes of stopping the calculation are excessive error indicated by the lack of energy conservation, penetration of the lattice, and "stalling" due to repeatedly reduced time increments demanded by the error control in the program.

We often observe several "bounces" from the surface region, each resulting in a decrease in particle energy. If the extended period of calculation is due primarily to the failure of the gas particle to move away from the surface, we call the state "trapped." Usually this trapping is due to a substantial energy loss to the lattice in the initial impact, although the particle may still retain enough total energy to give it the ultimate capability to climb out of the surface energy well. With each successive close approach to a surface atom additional energy is lost, and the possibility of the gas particle escaping before coming to equilibrium with the surface is further reduced.

We feel this trapping is a good indication of a state which would be temporarily absorbed in a real interaction and would therefore be totally accommodated to the actual surface state. We therefore assign to this molecule values of the output parameters corresponding to complete accommodation, and include it as such in the averaging for that state. The fraction trapped is indicated on the plots when applicable.

The other causes of stopping are much less frequent in our results. Stalling appears to have been completely eliminated by introducing a subroutine which backtracks and recalculates the earlier part of the trajectory with improved accuracy when a stall is encountered. In any event, the difficulty of performing the calculation as measured by the required number of calculation steps is strongly related to the strength of the interaction forces, which in turn are related to the degree of accommodation. Those states which display a significant number of trapped or uncalculatable trajectories usually indicate a high (i.e., > 0.6) energy accommodation for the remainder of the trajectories.

B. RESULTS OF THE STATISTICAL ANALYSIS

We are prevented by lack of space from listing the actual results from each of the 64 runs from our statistical design. These have been tabulated by Bogan (1964). The correlations given in Table II should be much more useful for most purposes. There are, in addition, a few general properties of the results that should be noted.

Perhaps the most hopeful indication in the data is that the azimuth angle φ_i is quite unimportant in the cases tested. This suggests that minor changes in type or orientation of crystal structure will probably also be unimportant, except as char-

acterized by changes in spacing. It is also of some interest to the experimenter, who faces the problem of controlled or preferential orientation of crystallographic planes.

A second strong indication is the importance of σ/d on the standard deviation of E_ℓ/E_i and on the level of σ_T and ψ . We can view σ/d as a measure of the roughness of the L-J potential surface, and as such it plays an important role in all scattering processes.

We find, as expected, that E_ℓ/E_i depends strongly on m_ℓ/m_g , Ω^2 , and D_w . There is also an important effect of θ_i , with a more glancing impact producing a smaller energy accommodation.

It is interesting to note that our balanced design appears to be reasonably well centered over the region in which large changes are taking place. The averages of E_ℓ/E_i and the other parameters are all quite near the midpoints of their respective ranges. The standard deviations of these properties have significant magnitudes, even for our "cold" lattice, averaging out to about 25 per cent of the means of the parameters themselves (σ_T is an exception due to a fair amount of back scattering contribution).

C. RESULTS OF SPECIFIC INTERACTIONS

In the group of calculations in which the gas and solid species are fixed, the number of independent input parameters is

reduced to 3; E_i , θ_i , and ϕ_i . We have chosen Ni as a solid and A, Ne, and He as gas species. Since our other work has indicated that ϕ_i is relatively unimportant, we have chosen $\phi_i = 15^\circ$, a condition without any particular symmetry, for all of these runs. The values for the physical constants for these interactions were taken from (or extrapolated from) those used by Goodman (1963), and are shown in Table III.

The mean results of 19 incident states, each represented by 18 trajectories, are shown in Figs. 6 and 7. Additional parameters and standard deviations are shown in Table IV. One can easily see the strong effects of mass ratio on energy accommodation, and (indirectly) on momentum exchange. The momentum coefficients depend more strongly on the exit energy than on any other effect present, suggesting that the spatial distributions of trajectories are relatively unchanged. The angles given in Table IV also indicate this characteristic.

It is important to note in interpreting these results that the net effect of incident energy is the result of two conflicting trends. The natural frequency parameter Ω^2 and the binding energy parameter D_w both decrease as E_i increases. From Table II we see Ω^2 has a negative influence and D_w has a positive influence on E_ℓ/E_i . These counteracting effects apparently combine to produce a minimum in E_ℓ/E_i . Such a minimum has also been indicated by the theory of Goodman (1963), although at much lower values of E_i .

VI. CONCLUSIONS

The results discussed above are of course limited by the assumptions in our model. There are many other effects that can enter the problem, and there is a corresponding need for other approaches, both theoretical and experimental. We expect to improve our model by including additional effects such as surface contaminants and roughness and to improve the present statistical and parametric analyses. From the present results, we feel the following conclusions are justified:

1. The use of independent lattice atoms (Einstein lattice) gives a reasonable approximation to the final gas particle energy throughout the dynamic range. Maximum errors are of the order of 10 per cent, occurring around $\omega_n \tau_c = 5$. They diminish to negligible values at both large and small values of $\omega_n \tau_c$.
2. The statistical prediction equations presented in Table II should be useful for many purposes. The predicted values show good agreement with the results of the specific-species interactions which often represent a considerable extrapolation of the original regions (especially in mass ratio). These correlations furnish

numerical predictions of many parameters of the exit distributions in terms of the input parameters and are relatively easy to use. The scatter in the predictions is quite low in terms of the present state of knowledge.

3. The statistical design appears to be quite satisfactory for our purposes. Originally set up to cover atmospheric gas species on engineering materials at hypervelocity conditions, the design has also turned out to be quite well centered over the region in which significant changes take place.
4. The two approaches discussed in this paper show trends whose direction and importance are explainable by physical reasoning. The trends in energy accommodation with mass ratio, binding energy and lattice natural frequency all show the kind of behavior that one would expect from the response of a mass-spring oscillator to the forces of a passing particle. Momentum coefficients show the expected effects of energy exchange and an additional dependence on the smoothness of the potential surface.

LIST OF SYMBOLS

A_{kj}	linear effect of x_j on α_k
B_{kj}	quadratic effect of x_j on α_k
COL	coupled oscillator lattice
d	unit of length ($= \frac{1}{2}$ lattice spacing)
D_w	dimensionless potential depth ($= \epsilon/E_i$)
E	energy
IOL	independent oscillator lattice
m	mass
r	distance between particle and surface
x_j	independent variable
V	velocity
α_k	dependent variable
$\alpha_{1D, (3D)}$	thermal accommodation coefficient for a one dimensional (three dimensional) lattice model
ϵ	depth of Lennard-Jones 6-12 potential
θ	angle between velocity vector and normal to surface
σ	range parameter of Lennard-Jones 6-12 potential
σ_T	tangential momentum accommodation coefficient
σ_z	normal momentum accommodation coefficient

τ_c	duration of a collision [Eq. (1)]
φ	azimuthal angle of velocity
ψ	angle between final ray and specular direction
ω	frequency
Ω	dimensionless frequency parameter $\left(= \omega_n \frac{d}{V_i}\right)$

Subscripts

c	collision
f	final state after interaction
g	gas
i	initial state
l	lattice (or solid)
n	natural frequency of lattice

Special Notation

$s(\alpha_k)$	standard deviation of α_k for 18 trajectories
\overline{F}	mean of F over 64 x 18 trajectories

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TABLE I
VALUES OF INPUT VARIABLES

Test Level	Ω^2	D_w	θ_i	m_ℓ/m_g	σ/d	ϕ_i
1	0.1	.001	120°	2.00	1.25	15°
2	1.00	.004	135°	4.00	1.50	30°
3	10.0	.016	150°			
4	100.0	.064	165°			
Center of Study Region	3.162	.008	142.5°	$\sqrt{8}$	1.375	22.5°

TABLE II

CORRELATION COEFFICIENTS FOR MEANS AND STANDARD DEVIATIONS OF INTERACTION PARAMETERS

	Grand Mean	$\ln(\Omega^2/\overline{\Omega^2})$		$\ln(D_w/\overline{D_w})$		$\theta_1 - \overline{\theta_1}$		$\ln\left(\frac{m_l/m_g}{m_l/m_g}\right)$	$\left(\frac{\sigma}{d}\right) - \overline{\left(\frac{\sigma}{d}\right)}$	$\varphi_1 - \overline{\varphi_1}$
		Linear	Quad	Linear	Quad	Linear	Quad	Linear	Linear	Linear
E_ℓ/E_1	.4662	-.0764*	-.0189*	.0590*	.0394*	.0039*		-.2259		
$s(E_\ell/E_1)$.1136	-.0074 [†]	-.0030*	.0016 [†]	.0087 [†]		-.0001	.0365 [†]	-.1671	
σ_z	1.7858	.0341*	.0055 [†]	-.1162*	-.0547*	-.0057*		.1678 [†]	-.1825 [†]	
$s(\sigma_z)$.4099			.0208*	.0121			.0961 [†]	-.2875	
σ_T	.6115	-.0086 [†]	-.0015 [†]	.0088 [†]	.0487*	.0068*		-.0541 [†]	-.7288*	
$s(\sigma_T)$.7298	.0573	.0099	-.0222	-.0081	.0205*		.3073 [†]	-.3461 [†]	
$\cos \theta_f$.6230	.0036*		-.0576*	-.0174*	.0047				
$s(\cos \theta_f)$.2325			.0260						
φ_f	34.16°				-1.963	.2383				.8664*
$s(\varphi_f)$	69.77°	2.007*		-4.5820*		1.7504*	-.0264*		-83.96	-.1157
ψ_f	36.09°	.7233				.4205*	-.0155*		-33.12*	
$s(\psi_f)$	16.76°	.3013	.0134	.7368	.8043	.1322	-.0060		-23.24	

NOTES: 1. Correlation format given in Eq. (2)

2. Significance levels: 0 - 90% — or .xxxx[†]
 90 - 99% .xxxx
 > 99% .xxxx*

TABLE III

ASSUMED L-J 6-12 INTERACTION PARAMETERS FOR (100) NICKEL SURFACE

Gas Species	ϵ (ev)	σ (A°)	m_g (AMU)
Argon	.0722	3.33	39.94
Neon	.0173	3.01	20.18
Helium	.00563	2.86	4.0

Nickel Data:

$$d = 1.76\text{\AA}^\circ \text{ (lattice half-spacing)}$$

$$\omega_n = .422 \times 10^{14} \text{ rad/sec}$$

$$m_\ell = 58.69 \text{ AMU}$$

TABLE IV
RESULTS FOR INERT GASES ON NICKEL
 (see also Figs. 6 and 7)

		$\overline{E_\ell/E_i}$	$s(E_\ell/E_i)$	$\overline{\sigma_z}$	$s(\sigma_z)$	$\overline{\sigma_T}$	$s(\sigma_T)$	$\overline{\cos \theta_f}$	$\overline{\varphi_f}$
<u>$\theta_i = 135^\circ$</u>									
Argon	0.125 ev	These runs are almost completely trapped.							
	0.5								
	2.0								
	4.0								
	8.0	.5702	.0920	1.5815	.2097	.1829	.0999	.4112	15.93
Neon	0.125	.5446	.1968	1.5775	.4981	.2712	.3794	.4084	21.85
	0.5	.4196	.1232	1.7247	.3993	.1936	.2598	.5124	18.00
	2.0	.3953	.1077	1.8913	.2544	.2179	.2292	.6303	18.28
	8.0	.4022	.1066	1.9667	.2496	.2898	.0259	.6836	20.76
Helium	0.125	.1315	.0484	1.8727	.09149	.2230	.4093	.6171	22.34
	0.5	.1132	.0398	2.0121	.2787	.2590	.3674	.7156	23.70
	2.0	.1170	.0401	2.0516	.2802	.3434	.4012	.7436	31.98
	8.0	.1292	.0460	2.0695	.2518	.4765	.4965	.7563	20.37
<u>$\theta_i = 165^\circ$</u>									
Argon	0.5 ev	Almost completely trapped.							
	2.0								
Neon	0.5	.6395	.1067	1.6925	.3176	.2506	.9786	.6689	22.29
	2.0	.6066	.0931	1.8316	.1380	.3346	.8912	.8033	23.55
Helium	0.5	.1764	.0378	1.8367	.1228	.3785	1.3636	.8082	45.22
	2.0	.1736	.0335	1.8234	.1332	.5378	1.4355	.7953	49.50

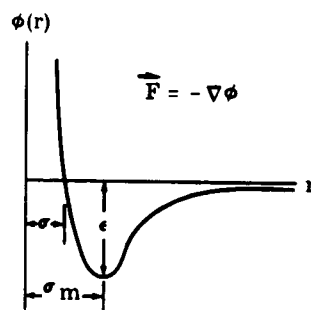


Fig. 1 Lennard-Jones 6-12 Potential

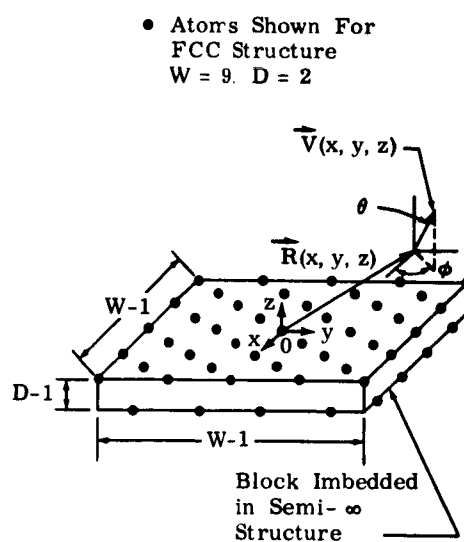


Fig. 2 Coordinate System and Lattice Atom Configuration for
Trajectory Calculations

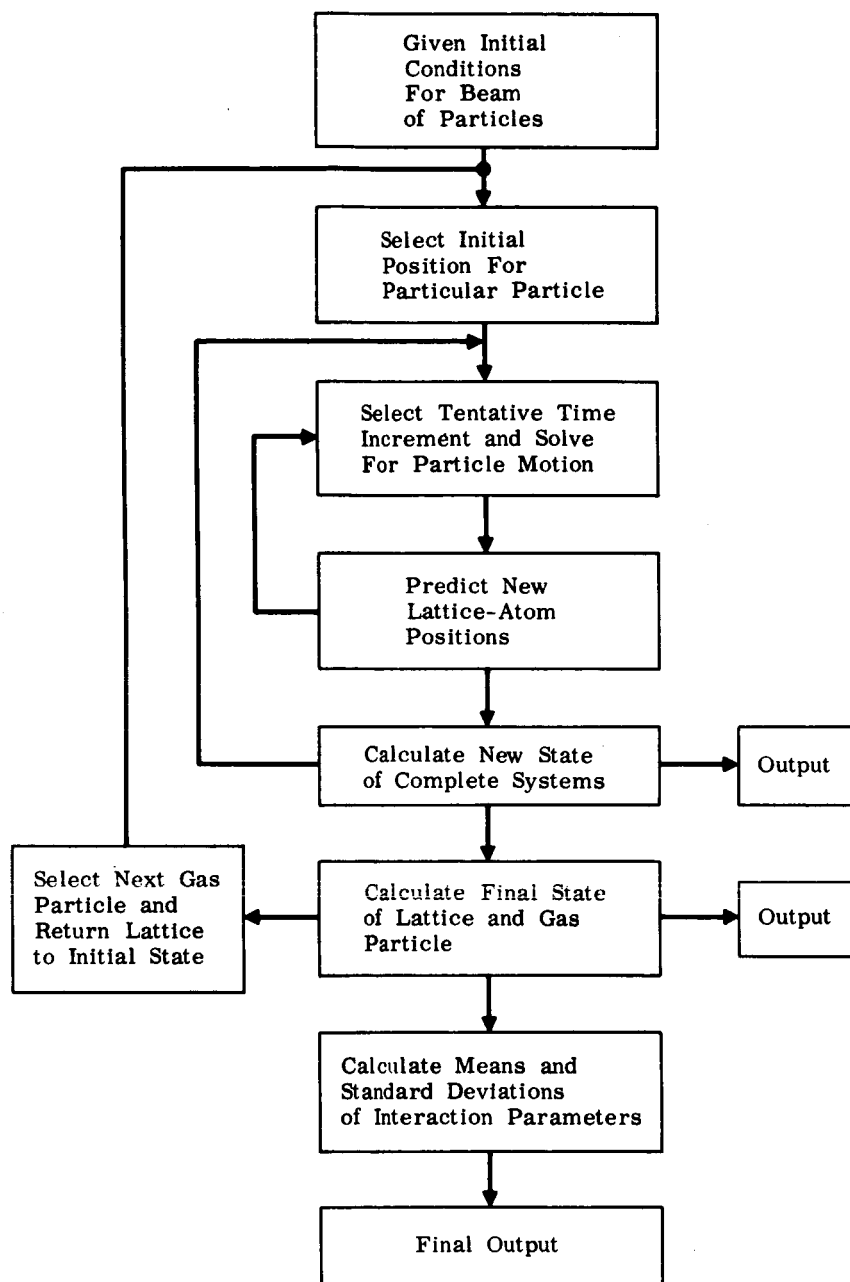


Fig. 3 Schematic Diagram of Computer Program Logic

a - Energy Accommodation

$$\Delta E = \frac{E_{fCOL} - E_{fIOL}}{E_i}$$

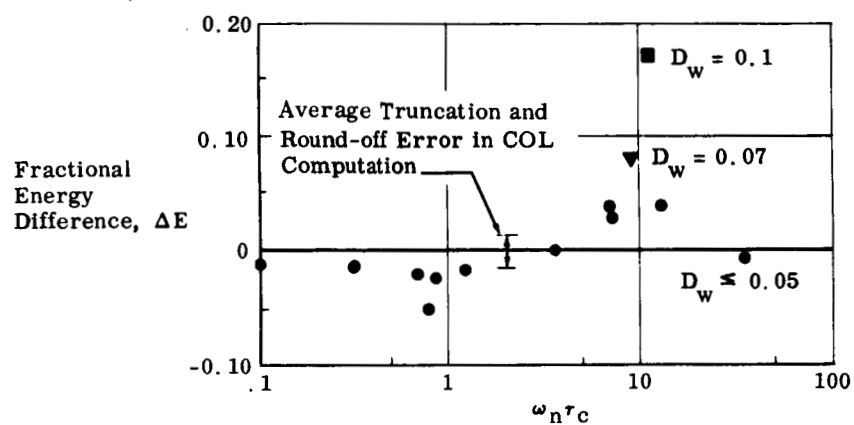


Fig. 4a Comparison Between Coupled-Oscillator and Independent-Oscillator Lattice Models

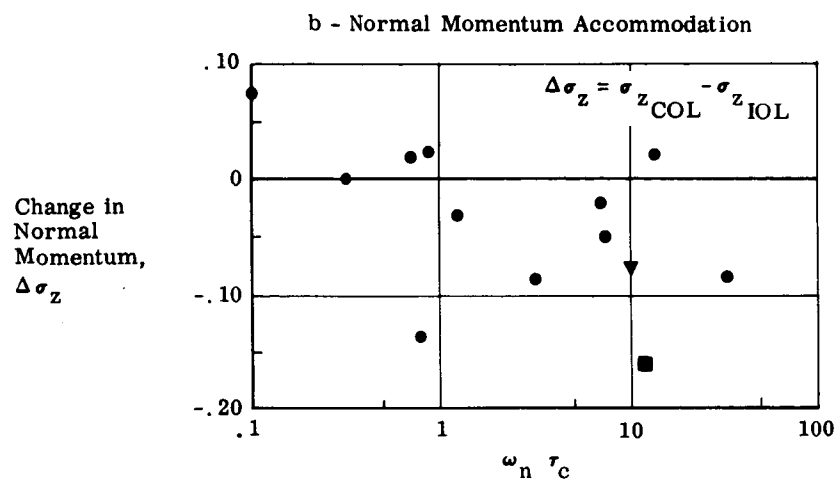


Fig. 4b Comparison Between Coupled-Oscillator and Independent-Oscillator Lattice Models

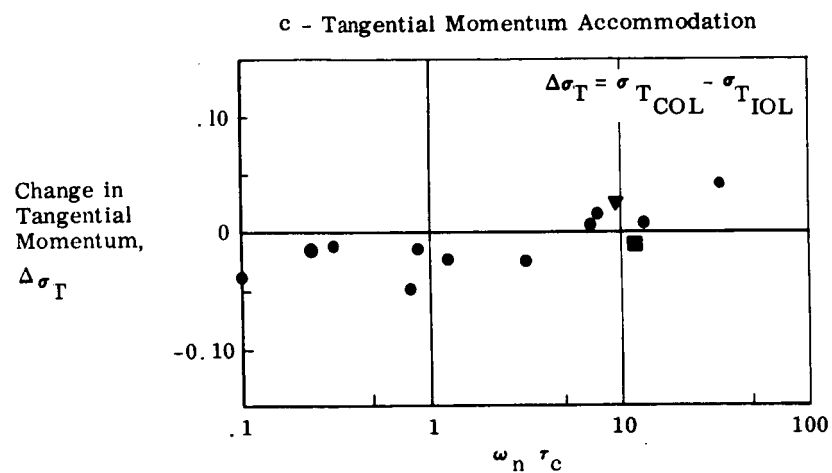


Fig. 4c Comparison Between Coupled-Oscillator and Independent-Oscillator Lattice Models

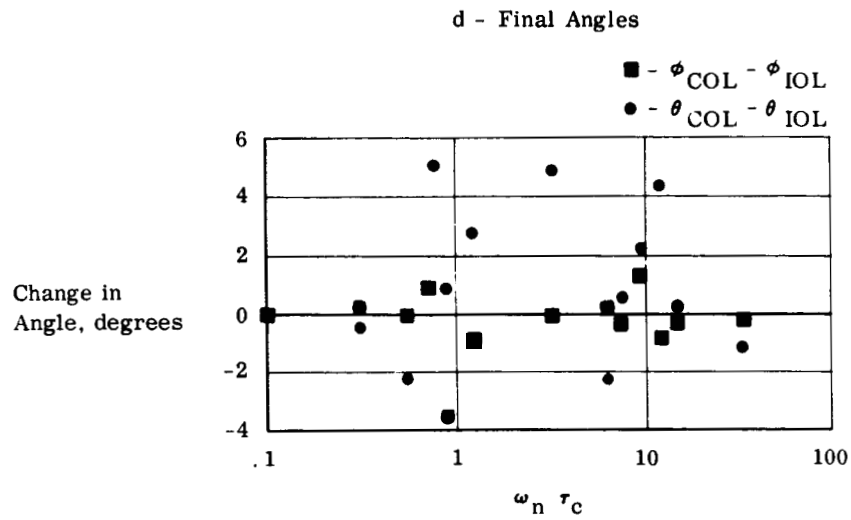


Fig. 4d Comparison Between Coupled-Oscillator and Independent-Oscillator Lattice Models

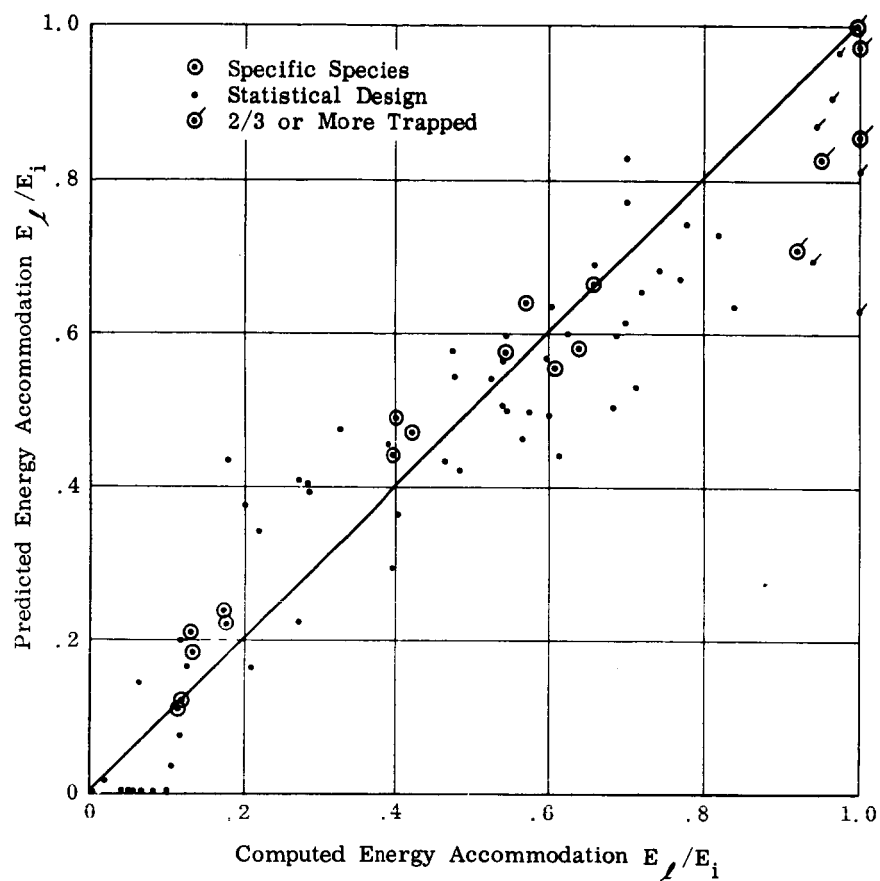


Fig. 5 Comparison of Calculated Energy Accommodation with Statistical Correlation

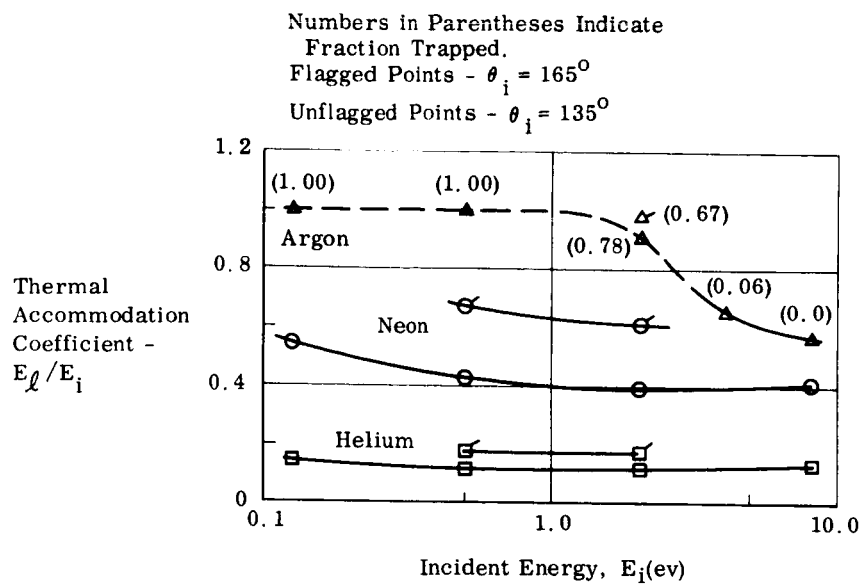


Fig. 6 Mean Thermal Accommodation for Inert Gases on Nickel

$$\text{--- Tangential, } \sigma_T \equiv \frac{\Delta V_T}{V_{T_i}} \quad \text{--- Normal, } \sigma_z \equiv \frac{\Delta V_z}{V_{z_i}}$$

Flagged - $\theta_i = 165^\circ$

Unflagged - $\theta_i = 135^\circ$

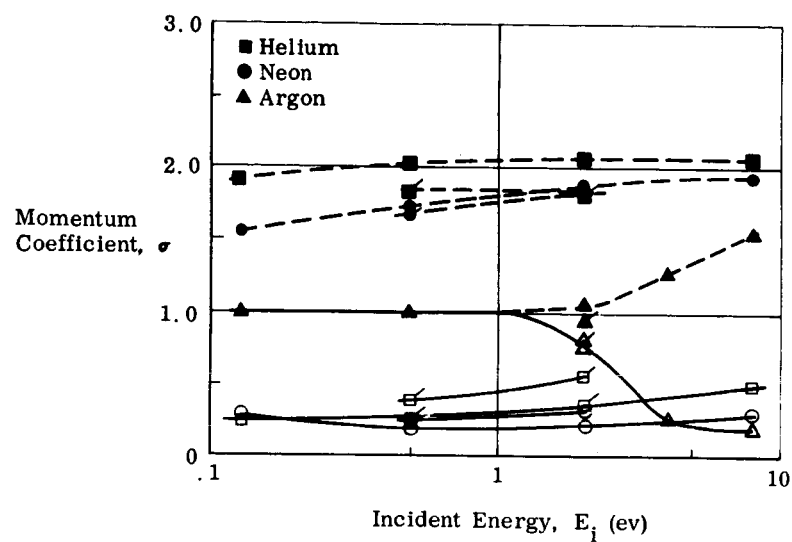


Fig. 7 Mean Momentum Accommodation for Inert Gases on Nickel